Syntheses of N-substituted 3,3,4-triphenyl-4-benzoylazetidin-2-ones and 3',3'-diphenyl spiro(acenaphthen-1-one-2,4'-azetidin-2'-ones); novel examples exhibiting a high

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reactivity of imino group in ketoimines

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S. B. SINGH and K. N. MEHROTRA. Can. J. Chem. 60, 1901 (1982).

The reaction of 2-diazo-1,2-diphenylethanone (1) with 2-imino-1,2-diphenylethanones 2a-e gave new N-substituted 3,3,4triphenyl-4-benzoylazetidin-2-ones 3a-e, together with 1,1',2,2'-tetraphenyl-2,2'-azinodiethanone (4). Similar reaction of 1 with 2-iminoacenaphthenones 6a, b yielded N-substituted 3',3'-diphenyl spiro(acenaphthen-1-one-2,4'-azetidin-2'-ones) 7a, b and ketazine 4. Lithium aluminium hydride reduction of azetidinones 3a, b gave 4α -hydroxybenzylazetidin-2-ones) 8a, b. The spiro azetidinones 3a-e and 7a, b were found to be unaffected by either acid or base hydrolysis. The marked selective reactivity of the imino group as compared to the carbonyl group towards diphenylketene has been observed in the present studies. The comparative reactivity of carbonyl groups present in azetidinones 3a, b and 7a, b has been presented.

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La diazo-2 diphényl-1,2 éthanone (1) réagit avec les imino-2 diphényl-1,2 éthanones (2a-e) en donnant les nouvelles triphényl-3,3,4 benzoyl-4 azétidinones-2 (3a-e) substituées sur l'azote ainsi que la tétraphényl-1,1',2,2' azino-2,2 diéthanone (4). D'une manière analogue, le composé 1 réagit avec les imino-2 acénaphténones (6a,b) en donnant les diphényl-3',3' spiro(acénaphténones-1 azétidine-2,4' ones-2') (7a,b) substituées sur l'azote ainsi que la cétazine (4). La réduction des azétidinones (3a,b) par LiAlH₄ conduit aux α -hydroxy benzyl-4 azétidinones-2 (5a,b). La réduction des spiro(azétidinones) (7a,b) par le borohydrure de sodium conduit aux spiro(hydroxy-1 acénaphtène-azétidine-2,4' ones-2') (8a,b). On a trouvé que les azétidinones (3a-e) et 7a,b) ne s'hydrolysent pas en milieu acide ou en milieu basique. Dans cette étude, on a observé une réactivité sélective marquée du groupe imino, par comparaison au groupe carbonyle, envers le diphénylcétène. On présente une comparaison de la réactivité des groupes carbonyles présents dans les azétidinones 3a,b et 7a,b.

[Traduit par le journal]

The cycloaddition of diphenylketene with imines (1), diimines (2), azines (3), conjugated imines (4), and 1,3-diazabutadienes (5) is known to form β -lactams. Addition of dimethylketene to 2-p-tolylimino-1,2-diphenylethanone, having a ketoimine group, has been observed to give 4,4-dimethyl-1,5diphenyl-2-p-tolyl-6-oxa-2-azabicyclo[3.1.0]hexan-3-one (6). A few spiro(2-azetidinones) have been obtained from the reaction of isocyanates with olefins (7) or allenes (8), carbodiimides with 4,4-dicarboxy-2-azetidinones (9), and acid chlorides with anils (10). We now report the cycloaddition of diphenylketene, generated in situ by thermal decomposition of 2-diazo-1,2-diphenylethanone (1), with 2-imino-1,2-diphenylethanones 2a-e and 2imino-acenaphthenones 6a, b leading to new azetidinones 3a - e and spiro azetidinones 7a, b in fair yields. This study has also revealed the marked selective reactivity of the imino group as compared to the carbonyl group in ketoimines 2a - e and 6a, b towards diphenylketene. The carbonyl group in the azetidinone ring in the products 3a-e and 7a, b is found to be unaffected either by hydrolysis or treatment with lithium aluminium hydride and

¹Revision received February 15, 1982.

sodium borohydride. The carbonyl group, not present in the azetidinone ring of the products 3a, b, is found to be less reactive than the corresponding carbonyl group in spiro azetidinones 7a, b as the former is reduced by lithium aluminium hydride while the latter is reduced even by sodium borohydride. Moreover, azetidinones 3a-e and 7a, bobtained in the present work could be used as precursors and their synthetic utility could be tapped as the carbonyl group left unattacked by diphenylketene could be developed to other desired functionalities.

Results and discussion

The product mixture obtained by the reaction of 2-diazo-1,2-diphenylethanone (1) with 2-isopropylimino-1,2-diphenylethanone (2a) was separated by fractional crystallization from *n*-hexane – ethanol (1:1) mixture and ethanol; it consisted of 1,1',2,2'tetraphenyl-2,2'-azinodiethanone (4, 4%) and 1isopropyl-3,3,4-triphenyl-4-benzoyl-2-azetidinone (3a, 44%). The structural assignment of 3a was made on the basis of analytical and spectral data given in Tables 1 and 2. The ir spectrum of 3a shows strong bands at 1740 (C=O, azetidinone) (11) and 1680 (C=O, benzoyl) cm⁻¹. The nmr

0008-4042/82/141901-06\$01.00/0

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			Product $3a-e$							
					Ele	mental A	Analysis (%)			
		Viold	Melting	Malagular		Found		Ca	alculated	 1
Ketoimines	R	(%)	(°C)	formula	C	Н	N	С	н	N
2 <i>a</i>	$\overline{CH(CH_3)}_2$	52	186-187	$C_{31}H_{27}NO_2$	83.18	6.45	2.96	83.59	6.06	3.14
2 b	$CH(C_6H_4 - p - CH_3)CH_3$	31	155-156	$C_{37}H_{31}NO_{2}$	84.72	6.20	3.22	85.22	5.96	2.68
2 c	CH(Ph)CH ₃	44	176-177	$C_{36}H_{29}NO_2$	85.31	5.31	3.01	85.20	5.72	2.76
2 d	CH(Ph),	11	198–199	$C_{41}H_{31}NO_2$	86.90	5.47	2.77	86.46	5.45	2.46
2 e	Ph	47	177-178	$C_{34}H_{25}NO_2$	84.96	5.40	2.97	85.18	5.22	2.92

TABLE 1. CONVERSION OF RECOMMENDS $2u - e$ to accumulates $3u$.	TABLE	1.	Conversion	of ketoimines	2a - e to	azetidinones	3a - b
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spectrum of 3*a* displays the aromatic protons as multiplets at δ 7.33 (15H) and 6.97 (5H), the methine proton as a septet at δ 3.48 (J = 7 Hz) and the methyl protons as a pair of doublets (11) at δ 1.70 and 1.23 (6H, J = 7 Hz). The mass spectrum shows the molecular ion peak at m/e 445. The authentic sample of 4 was prepared according to the reported method (12) for comparison (ir, nmr, and also mmp).

Similar treatment of ketoimines 2b-e with 1 gave azetidinones 3b-e (11-45%), identified on the basis of their analytical and spectral (uv, ir, and nmr) data (Tables 1 and 2), and ketazine 4 (5-10%).

The reduction of 3a with lithium aluminium

hydride in dry ether gave 1-isopropyl-3,3,4-triphenyl-4-(α -hydroxybenzyl)-azetidin-2-one (5*a*, 86%), characterized on the basis of analytical and spectral data. Its ir spectrum exhibits a medium intensity band at 3440 cm⁻¹, characteristic of the O—H group, and a strong band at 1735 cm⁻¹, characteristic of C=O (azetidinone) (11). The nmr spectrum displays the aromatic protons as multiplets at δ 7.93 (2H), 7.53 (4H), and 7.05 (14H), the benzylic proton as a doublet (collapses to a singlet on deuteration) at δ 4.89 (J = 4 Hz), the methine proton as a septet at δ 2.69 (J = 7 Hz), the hydroxy proton as a broad singlet at δ 2.00 (exchangeable on deuteration), and the methyl protons as a pair of



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doublets (11) at δ 1.54 and 1.20 (6H, J = 7 Hz). When the product 3b was treated with LAH in a similar way, the reduced product 5b was obtained. The formation of products 3a-e, 4, and 5a, b is shown in Scheme 1.

2-Imino-acenaphthenones 6a, b were prepared by the condensation of appropriate amines with acenaphthenequinone in dry toluene; ir (Nujol): 1730 (C=O, quinone) (13) and 1650 (C=N) cm⁻¹; uv (ethanol): 228, 305, 365, and 440 nm. The nmr spectra are in agreement with the proposed structures.2

The reaction between 1 and 2-phenylimino-acenaphthenone (6a) gave ketazine 4 and 1', 3', 3'-triphenyl spiro(acenaphthen-1-one-2,4'-azetidin-2'one) (7*a*). The product 7*a* shows absorption maxima at 250, 318, and 345 nm in the uv spectrum. The ir spectrum exhibits strong bands at 1750 and 1730 cm⁻¹, characteristic of a spiro azetidinone (10) and a quinone (13), respectively. The sodium borohydride reduction of 7a afforded 1',3',3'-triphenyl spiro(1-hydroxyacenaphthene-2,4'-azetidin-2'one)(8a); ir (neat): 3580 (O-H), 1750 (C=O, spiro azetidinone) cm^{-1} and absence of a band at 1730 cm^{-1} , characteristic of a quinone (13), revealing that the reduction of the carbonyl group at the 1-position of 7a has occurred. Similar treatment of 1 and 6b gave spiro azetidinone 7b, which on reduction with sodium borohydride gave 8b and ketazine 4. The products 7a, b have been characterized by analytical and spectral (uv, ir, and nmr) data given in Tables 3 and 4. The formation of products 7a, b and 8a, b is depicted in Scheme 2.

The azetidinones 3a-e and spiro azetidinones 7a, b were found to be resistant to ordinary alkaline or acid hydrolysis supporting the above assigned structures. The bicyclic product, obtained earlier (6) by reaction of dimethylketene and 2-p-tolyl imino-1,2-diphenylethanone, undergoes hydrolysis quite readily (6).

Thermal decomposition of 2-diazo-1,2-diphenylethanone (1) may lead to benzovlphenylcarbene which may combine with 1 to form ketazine 4. Benzoylphenylcarbene has been known to undergo Wolff rearrangement to give rise to diphenylketene (14) which may interact either with the C=N bond (15) or with the C=O (16) of ketoimines 2 and 6 leading to either azetidinones or β -lactones. The β -lactones, on decarboxylation, would have readily given rise to the corresponding olefins (16). The formation of azetidinones and not β -lactones has been supported on the basis of the analytical,

		TABLE 2. 5	Spectral data of	azetidinones	3a−e	
		Ultraviolet	Infrared (Nuj	jol) (cm ⁻¹)	Nuclear mag	metic reconsarce (CDCI) 8 (nnm)
		λ _{max} (EtOH)	v (C==0)	v (C=0)		
Azetidinones	R	(uu)	azetidinone	benzoyl	Aromatics	Others
3a	CH(CH ₃) ₂	230	1740	1680	7.33 (15H), 6.97 (5H)	3.48 (sept, 1H, methine, isoprop) J = 7 Hz), 1.70 and 1.23 (a pai of doublets, 6H, CH ₃ isopropy J = 7 Hz)
3b	CH(C ₆ H ₄ <i>p</i> -CH ₃)CH ₃	255	1740	1680	7.63 (4H), 7.28 (8H), 6.92 (12H)	4.44 (q, 1H, methine, α -tolylethy J = 7 Hz), 2.25 (s, 3H, CH,, $ptolyl), 2.17 (d, 3H, CH,, \alpha-tolylethyl, J = 7 Hz)$
3 c	CH(Ph)CH ₃	230	1745	1680	7.42 (20H), 6.79 (5H)	4.17 (q, 1H, methine, α -phenyl- ethyl, $J = 7$ Hz), 1.61 (d, 3H, CH ₃ , α -phenylethyl, $J = 7$ Hz
3d	$CH(Ph)_2$	255	1740	1680	7.42 (30H)	5.53 (s, 1H, methine, benzhydry)
3e	Ph	250	1750	1670	7.36 (H)	

²Microanalyses for C, H, N are satisfactory, maximum error for C, \pm 0.40; H, \pm 0.20, N, \pm 0.24.

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				1	Product 7	a,b				
						Ele	mental A	Analysis (%)	
		Viald	Melting	Mologular		Found		Ca	alculated	1
Ketoimines	R	(%)	(°C)	formula	С	Н	N	С	н	N
6a 6b	Ph C_6H_4 — p -CH ₃	76 72	235–236 175–176	$\begin{array}{c} C_{32}H_{21}NO_2\\ C_{33}H_{23}NO_2 \end{array}$	85.41 84.97	4.88 4.80	3.18 3.01	85.14 85.16	4.66 4.95	3.10 3.01

TABLE 3. Conversion of ketoimines 6a, b to spiro azetidinones 7a, b

TABLE 4. Spectra	l data of spire	o azetidinones	57a,	Ł
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		Ultraviolet	Infrared (Nuj	ol) (cm ⁻¹)	
Spiro azetidinones	R	λ_{max} (EtOH) (nm)	v (C==O) (azetidinone)	v (C=O) (quinone)	Nuclear magnetic resonance (CDCl ₃) δ (ppm)
7 a	Ph	250, 318, 345	1750	1730	8.17 (m, 4H, arom.), 7.25 (m, 16H, arom.), 6.67 (d, 1H, arom., <i>J</i> = 7 Hz)
7 b	C ₆ H ₄ —p-CH ₃	255, 318, 345	1750	1730	7.98 (m, 4H, arom.), 7.28 (m, 11H, arom.), 6.85 (m, 3H, arom.), 6.59 (m, 2H, arom.), and 2.13 (s, 3H, CH ₃)



$$b \quad Ar = C_6 H_4 - p - CH$$



Scheme 2

spectral, and chemical behaviour of the products. This reaction shows the high reactivity of the C=N in comparison with the C=O group towards diphenylketene. Since azetidinones 3a-e show their inertness towards sodium borohydride while the spiro azetidinones 7a, b undergo reduction with sodium borohydride, the carbonyl group present in the benzoyl moiety of azetidinones 3a-e is less reactive than the quinone carbonyl group of spiro azetidinones 7a, b. The azetidinone ring in 3a-e

and 7a, b is unaffected on reduction (NaBH₄ or LiAlH₄) and thus appears to be quite stable. The formation of azetidinones takes place through the collapse of a possible zwitterionic intermediate (Scheme 3). A similar intermediate has been proposed in the reaction of diphenylketene and benzyl-ideneaniline giving N-phenylimidate (15).

Experimental

Melting points were determined on a Büchi apparatus (capillary method) and have been uncorrected. Ultraviolet spectra were obtained in 95% ethanol on a Cary-14 spectrophotometer. Infrared spectra were recorded in Nujol mull on a Perkin–Elmer 720 spectrophotometer. Proton nuclear magnetic resonance data were obtained on a Varian A-60D spectrometer in CCl₄ or CDCl₃ using TMS as internal standard.

Materials

Benzil, lithium aluminium hydride, and sodium borohydride were obtained from EGA chemicals, West Germany and 2-diazo-1,2-diphenylethanone (17), α -phenylethylamine (18), α -p-tolylethylamine (18), benzhydrylamine (19), and acenaphthenequinone (20) were prepared according to the reported methods.

General procedure for preparation of ketoimines 2a-e and 6a, b

The ketoimines 2a-d were prepared by dissolving a mixture containing 10 mmol of benzil and 10 mmol of corresponding freshly distilled amine in 30-40 mL of absolute ethanol at room temperature and keeping it for a week. The ketoimines 6a, b were obtained by refluxing a solution of 10 mmol of acenaphthenequinone and 10 mmol of corresponding amine in 60-80 mL of dry toluene for 2 h using a Dean-Stark separator to remove the water formed. The ketoimine 2e was obtained by heating a mixture of equimolecular amounts of benzil and aniline at 150°C for 2 h. The solvent in all cases was removed on a rotary evaporator and residual matter was triturated with ethanol. The

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SCHEME 3

solid obtained was crystallized from ethanol to afford the product.

General procedure for preparation of azetidinones 3a-e and spiro azetidinones 7a, b

A mixture containing 10 mmol of 2-diazo-1,2-diphenylethanone (1) and 10 mmol of ketoimines 2a-e or 6a, b in 80 mL of dry benzene (thiophene free) was heated to reflux for 8 h under a nitrogen atmosphere. The reaction mixture was kept overnight at room temperature. The solvent was evaporated on a rotary evaporator and the residual matter was triturated with ethanol. The solid obtained was crystallized from ethanol to afford the products. The analytical and spectral data of the products 3a-e and 7a, b have been given in Tables 1-4. Evaporation of solvent from the mother liquor and crystallization from a *n*-hexane – ethanol (1:1) mixture gave a yellow crystalline solid identified as 1,1',2,2'-tetraphenyl-2,2'-azinodiethanone (4) on the basis of comparison (undepressed mixture melting point and identical ir spectrum) with an authentic sample prepared according to the reported method (12).

Attempted hydrolysis of azetidinones 3a-e and spiro

azetidinones 7a, b

A mixture containing 0.02 g of 3a, 15 mL of 85% ethanol, and 1 mL of concentrated hydrochloric acid was heated to reflux for 30 h. After the usual work-up, 0.18 g (90%) of starting material was recovered. Similar treatment of 3b-e with concentrated HCl and 3a-e and 7a, b with either 40% aqueous alkali (potassium hydroxide or sodium hydroxide) or saturated ethanolic potassium hydroxide solution resulted in the recovery of starting material almost quantitatively.

Preparation of 1-isopropyl-4-(α-hydroxybenzyl)-3,3,4-triphenyl-2-azetidinone (5a)

To a suspension of 0.10 g of lithium aluminium hydride in 10 mL of dry ether was added slowly a solution of 0.23 g of 3a in 20 mL of dry ether. The reaction mixture was stirred for 3 h and kept overnight at room temperature. After the usual work-up, an

oily material was obtained which on crystallization from ethanol gave 0.20 g (89%) of 5*a*; mp 177–178°C; ir (Nujol): 3440 (O—H) and 1735 (C==O, azetidinone) cm⁻¹; ν_{max} (ethanol): 255 nm; nmr (CCl₄) δ : 7.93 (m, 2H, arom.), 7.53 (m, 4H, arom.), 7.05 (m, 14H, arom.), 4.89 (d, 1H, benzylic, J = 4 Hz, collapses to a singlet on deuteration), 2.69 (septet, 1H, isopropyl, J = 7 Hz), 2.00 (b, 1H, OH, D₂O exchangeable), 1.54 and 1.20 (a pair of doublets, 6H, isopropyl, J = 7 Hz). *Anal*. calcd. for C₃₁H₂₉NO₂: C 83.22, H 6.49, N 3.13; found: C 83.40, H 6.55, N 3.25.

Preparation of 1-(α -p-tolylethyl)-3,3,4-triphenyl-4-(α -hydroxybenzyl)-azetidin-2-one (5b)

Treatment of 0.26g of 3b and 0.10g of lithium aluminium hydride in a similar manner as described above gave 0.22 g(85%) of 5b, mp 75–76°C; ir (Nujol): 3400 (O—H) and 1730 (C=O, azetidinone) cm⁻¹; uv_{max} (ethanol): 258 nm; nmr (CDCl₃) \delta 8.12 (m, 2H, arom.), 7.23 (m, 22H, arom.), 5.03 (s, 1H, benzylic), 3.33 (q, 1H, methine, J = 7 Hz), 2.33 (s, 3H, CH₃—p-C₆H₄—), 2.33 (s, 1H, OH, D₂O exchangeable), and 1.72 (d, 3H, methyl, J = 7 Hz). Anal. calcd. for C₃₇H₃₃NO₂: C 84.89, H 6.31, N 2.67; found: C 84.65, H 6.21, N 2.71.

Preparation of 1',3',3'-triphenyl spiro(1-hydroxyacenaphthene-2,4'-azetidin-2'-one) (8a)

To a solution of 0.20 g of 7*a* in 20 mL of absolute ethanol (acetaldehyde free), 0.10 g of sodium borohydride was added. The reaction mixture was stirred for 30 min and kept overnight. After the usual work-up, 0.18 g (90%) of a white oily product 8*a* (which could not be further purified) was obtained; ir (neat): 3580 (O—H) and 1750 (C==O, azetidinone) cm⁻¹; the ir spectrum does not show a band at 1730 cm⁻¹, characteristic of quinone (13).

Preparation of 1'-(p-tolyl)-3',3'-diphenyl spiro(1-hydroxy-

acenaphthene-2,4'-azetidin-2'-one) (8b)

Treatment of 0.20 g of 7b with 0.10 g of sodium borohydride in a similar manner as described above gave 0.18 g (90%) of a white oily product **8***b* (which could not be further purified); ir (neat):

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3520 (O—H) and 1750 (C=O, azetidinone) cm⁻¹. The ir spectrum does not show a band at 1730 cm^{-1} , characteristic of a quinone (13).

Acknowledgements

We thank Professor B. M. Shukla for providing facilities and the Council of Scientific and Industrial Research, New Delhi, India for grant of a fellowship to S.B.S.

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ADDITIONS AND CORRECTIONS/AJOUTS ET CORRECTIONS

Vol. 59, 1981

John T. Edward. Conformational effects on the enthalpy of formation of straight and branched-chain alkanes.

Page 3192. Professor P. v. R. Schleyer has brought to my attention that the essential arguments of the paper are to be found in the paper by P. v. R. Schleyer, J. E. Williams, and K. R. Blanchard, "The evaluation of the strain in hydrocarbons. The strain in adamantane and its origin" (J. Am. Chem. Soc. 92, 2377 (1970)). The group increments for "skew-free conformations" calculated by Schleyer *et al.*, in kcal/mol, are as follows (corresponding values of Edward follow in parentheses): CH₃,

 $-10.05~(-10.06);~CH_2,~-5.13~(-5.13);~CH,~-2.16~(-2.14);~C,~-0.30~(-0.11).$ I regret overlooking Professor Schleyer's paper.

J. M. Stadlbauer, B. W. Ng, D. C. Walker, Y. C. Jean, and Y. Ito. Muonium addition to vinyl monomers.

Page 3261. (i) The value of $k_{\rm H}$ in Table 2 should be 4×10^9 not $4 \times 10^{10} M^{-1} {\rm s}^{-1}$; and (ii) a_{μ} should have been used for the hyperfine coupling constant on line 13 of p. 3263, rather than A_{μ} which is the muon asymmetry in eq. [1].